Amendments to the Claims

Claim 1 (Currently Amended): A computer-aided method for the provision~~,~~ and identification ~~and description~~ of molecules exhibiting a desired activity comprising;

a molecular modeling step in which molecular descriptors are selected computationally;

a step of building a combinatorial library of molecules;

a step of selecting candidate molecules from the combinatorial library which potentially exhibit said desired activity;

a filtering step whereby the candidate molecules are filtered using at least one static filter representing a plurality of said molecular descriptors which each candidate molecule must satisfy in order to exhibit said desired activity; and

a further filtering step whereby the filtered candidate molecules are further filtered using at least one dynamic filter representing constraints of conformational variations which each candidate molecule must satisfy in order to exhibit said desired activity;

wherein the filtering steps allow for the identification of molecules exhibiting said desired activity.

Claims 2-8 (Cancelled)

Claim 9 (Currently Amended): A computer-aided method according to Claim ~~5 or Claim 8~~ 1 wherein ~~at least one of~~ said dynamic ~~criteria~~ filter is based on a shape descriptor derived from a 3 D autocorrelation vector (3D-ACV) ~~of the candidate molecule~~.

Claim 10 (Currently Amended): A computer-aided method according to Claim 9 wherein the static ~~criteria are~~ filter is based on physiochemical and topological descriptors at least some of which are chosen from the following descriptors: Molar Mass; Ellipsiodal Volume; Molecular Volume; Molar

Refractivity; Lipophilia (LogP); Kappa 1; Kappa 2; Kappa 3; Kappa Alpha 1; Kappa Alpha 2; Kappa Alpha 3; Flexibility; Kier Chi V4; Randic Index; Balaban Index; Weiner Index; Sum of Condition E; Dipolar Moment; Number of C Atoms; Number of O Atoms; Number of N Atoms; Number of H Atoms; Total Number of Atoms; Number of Methyl Groups; Number of Ethyl Groups; Number of Amino Groups; Number of Hydroxyl Groups.

Claims 11-17 (Cancelled)

Claim 18 (Currently Amended): A computer-aided method for the provision~~,~~ and identification ~~and description~~ of molecules exhibiting immunomodulatory activity comprising;

a step of molecular modeling in which molecular descriptors of a molecule having immunomodulatory activity are selected computationally;

a step of building a combinatorial library including molecules having said immunomodulatory activity;

a step of selecting candidate molecules from the combinatorial library which are potentially immunomodulatory;

a filtering step whereby the candidate molecules are filtered using at least one static filter representing a plurality of said molecular descriptors which each candidate molecule must satisfy in order to exhibit said immunomodulatory activity; and

a further filtering step whereby the filtered candidate molecules are further filtered using at least one dynamic filter representing constraints of conformational variations which each candidate molecule must satisfy in order to exhibit said immunomodulatory activity;

wherein the filtering steps allow for the identification of molecules exhibiting said immunomodulatory activity.

Claim 19 (Original): A computer-aided method according to claim 1 wherein the combinatorial library building step

comprises building a combinatorial peptide library.

Claim 20 (Original): A computer-aided method according to claim 1 wherein the combinatorial library building step comprises building a combinatorial peptoid library.

Claims 21-72 (Cancelled)

Claim 73 (Currently Amended): A computer-aided method according to Claim [[5]] 1 wherein the static ~~criteria are~~ filter is based on physiochemical and topological descriptors at least some of which are chosen from the following descriptors: Molar Mass; Ellipsiodal Volume; Molecular Volume; Molar Refractivity; Lipophilia (LogP); Kappa 1; Kappa 2; Kappa 3; Kappa Alpha 1; Kappa Alpha 2; Kappa Alpha 3; Flexibility; Kier Chi V4; Randic Index; Balaban Index; Weiner Index; Sum of Condition E; Dipolar Moment; Number of C Atoms; Number of O Atoms; Number of N Atoms; Number of H Atoms; Total Number of Atoms; Number of Methyl Groups; Number of Ethyl Groups; Number of Amino Groups; Number of Hydroxyl Groups.